

chain nodes :

17 18

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 19

chain bonds :

10-17 17-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-19 5-6 5-8 7-9 7-8 7-19 8-12 9-10 10-11
11-12

exact/norm bonds :

4-19 5-8 7-19 10-17 17-18

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-9 7-8 8-12 9-10 10-11 11-12

G1:Cl,F

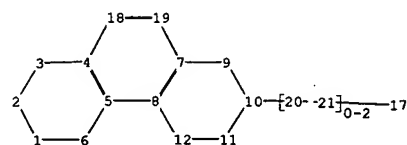
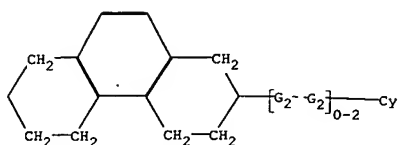
G2:C,O,N

G3:C,O,S,N

G4:C,H,Cl,F,CF₂,CF₃

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 17:Atom 18:CLASS 19:Atom



chain nodes :

17 20 21

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 18 19

chain bonds :

10-20 17-21 20-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-18 5-6 5-8 7-9 7-8 7-19 8-12 9-10 10-11
11-12 18-19

exact/norm bonds :

1-2 1-6 2-3 3-4 5-6 7-9 8-12 9-10 10-11 10-20 11-12 17-21 20-21

normalized bonds :

4-5 4-18 5-8 7-8 7-19 18-19

G1:Cl,F

G2:C,O,N

G3:C,O,S,N

G4:C,H,Cl,F,CF2,CF3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS